

The Possibility of Existence of an Energy Gap in the One-Particle Excitation Spectrum of He II

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Possibility for coexistence of a phonon and one-particle spectra in ^4He at all temperatures including temperatures below the λ - point is shown. An approach developed to consider the problem of the weakly imperfect Bose gas results in the existence of a gap in the one-particle (one-atom) excitation spectrum below the transition point. Thus, the microscopic model of He II turns out to differ both from the model initially suggested by Landau and from the Bogolyubov model accepted at present. Analysis of the experimental data obtained by measuring enthalpy and the part of helium atoms condensed in the state with the momentum $p = 0$ enabled to estimate the size of the gap. It turned out to be approximately equal to 0.31 K at zero temperature.

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I. INTRODUCTION

It is generally accepted that the superfluidity (SF) of He II was explained by to L.D.Landau in 1941. Less known is the fact that Landau initially assumed the existence of two branches in the excitation spectrum of the system: phonon and roton branches. At that, the latter corresponded to quanta of rotational degree of freedom of the liquid and was separated from the ground state by an energy gap.

However, subsequently a viewpoint based, in particular, on the work of Bogolyubov [1] was accepted. It assumes that only one phonon - roton excitation spectrum exists at zero temperature. We think that it is more correct to refer

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to it as one-particle (one-atom), because it is believed that the creation and annihilation of phonons cannot lead to a change in the number of atoms of the system, while the creation and annihilation operators for the so-called bogolons do not commute with the total number of particles in the system. In particular, as a result, the basic Hamiltonian of the system obtained by the Bogolyubov transformation does not preserve the total number of atoms. This fact, however, is ignored by all the authors: it is considered to be just a consequence of the so-called spontaneous breaking of symmetry of the system due to the presence of a second order phase transition.

This variant of describing the energy spectrum creates a number of questions. On one hand, naturally, no one doubts the coexistence of phonon and one-atom spectra at temperatures above the transition point [2]. So, there should be a mechanism of disappearance of one of the excitation branches below the transition point. According to the conventional point of view the disappearance of the phonon branch occurs immediately after the appearance of a macroscopic occupation number of the lower level of the system [2]. What experimentalists consider to be a spectrum of phonons, strictly speaking, as we mentioned above, is already a one-atom excitation spectrum, although it is characterized by a linear relationship between the excitation frequency and the wave vector in the long-wave limit. Therefore, a gigantic hysteresis of the transition temperature should exist in the system, because it is obvious that the transition point in a boson system with one-atom spectrum corresponding to the experimental phonon - roton spectrum of He II should considerably exceed the value corresponding to the parabolic spectrum of the system accepted for temperatures above the transition point. In this connection it is pertinent to remind that, according to the Landau theory, excitations of the phonon - roton branch form a normal component in the two-fluid model of He II.

In discussing this problem, the systematic research on numerical modelling of the properties of He II in the temperature range where the system heat capacity considerably differs from the phonon - roton gas heat capacity would be extremely interesting and desirable. However, unfortunately, we do not know works in this direction.

Quite recently the questions, concerning the concept itself of spontaneous breaking of symmetry in the considering context, also appeared [3]. The point is that the total number of atoms in the system is not preserved only in case of the truncated Hamiltonian, in which only the expressions bilinear with respect to the creation and annihilation operators of bogolons are selected. As for the total Hamiltonian of the system, of course, it does not break any symmetry. From this point of view the symmetry breaking is rather mathematical in nature and associated with the approximations inherent in the method used for calculating the wave functions of the ground state and low-energy excitations. But on the physical level, there is no symmetry breaking. If one does not take this into account, a paradox [3] results, which until now has not been considered in the works concerning the description of the weakly imperfect Bose gas as a qualitative model for the consideration of physical processes in He II in the standard SF theory (of course, we assume that the BCS - Bogolyubov theory of superconductivity is obviously associated with the Landau - Bogolyubov SF theory).

Two possible options for further research are possible. On one hand, one can try to prove that solving this paradox

does not affect the final results of calculations of He II within the framework of the microscopic Bogolyubov theory. This method seems to be very attractive, because a large number of experimental data were described in the context of the standard approach (at least qualitatively).

On the other hand, we think that it is very interesting to focus efforts on another method: a search of options for describing the system, which would maintain strictly the fundamental symmetries of the system at all steps of considering it. It is in the search for such an approach that we undertook this study. It will be shown below that it suggests a different scheme of the excitations branches in He II.

II. THE ALTERNATIVE PERTURBATION THEORY IN THE MODEL OF WEAKLY IMPERFECT BOSE GAS

First, note that the result presented in this section was obtained by Bogolyubov [4], if to limit to its mathematical part. The limitation concerning the mathematical part is not accidental. It is caused by the fact that, when Bogolyubov obtained a gap in the spectrum of quasiparticles, he rejected this solution on the basis of his concept of the physical properties of the system. We will discuss this item later.

So, let us consider spinless bosons (^4He atoms) with interatomic interaction $V(r)$ as a system located in the box $L_x \times L_y \times L_z$. We will assume that the boundary conditions of the system are periodical. Then the Hamiltonian of the system \hat{H} in the model of the the weakly imperfect Bose gas [4] has the form:

$$\begin{aligned}\hat{H} &= \hat{T} + \hat{V}, \\ \hat{T} &= \sum_{\mathbf{p}} t_{\mathbf{p}} b_{\mathbf{p}}^+ b_{\mathbf{p}}, \\ \hat{V} &= \frac{1}{2} \Omega^{-1} \sum_{\mathbf{p}, \mathbf{k}, \mathbf{q}} V_{\mathbf{q}} b_{\mathbf{p}+\mathbf{q}}^+ b_{\mathbf{k}-\mathbf{q}}^+ b_{\mathbf{k}} b_{\mathbf{p}},\end{aligned}\tag{1}$$

where $t_{\mathbf{p}} = \frac{p^2}{2M}$, M is the atomic mass of ^4He , Ω is the system volume, $V_{\mathbf{q}} = \int V(r) \cos(\mathbf{q}\mathbf{r}) d\mathbf{r}$, $b_{\mathbf{p}}^+$ and $b_{\mathbf{p}}$ are the creation and the annihilation operators for ^4He atoms in a state with a momentum \mathbf{p} .

Let us calculate the one-atom energy $\tilde{t}_{\mathbf{p}}$ of the ^4He atoms using an equation based on a random phase approximation (RPA) $[\hat{H}, b_{\mathbf{p}}^+] = \tilde{t}_{\mathbf{p}} b_{\mathbf{p}}^+$. Let us select first the diagonal part of the Hamiltonian \hat{H}_{diag} , because only this part is important for this calculation. For \hat{H}_{diag} we easily obtain:

$$\hat{H}_{diag} = \hat{T} + \frac{1}{2} \Omega^{-1} \sum_{\mathbf{p}, \mathbf{k}} \frac{V_0 + V_{\mathbf{k}-\mathbf{p}}}{1 + \delta_{\mathbf{p}}^{\mathbf{k}}} b_{\mathbf{p}}^+ b_{\mathbf{k}}^+ b_{\mathbf{k}} b_{\mathbf{p}},\tag{2}$$

where $\delta_{\mathbf{p}}^{\mathbf{k}}$ is the three-dimensional Kronecker symbol. Denominator $1 + \delta_{\mathbf{p}}^{\mathbf{k}}$ was introduced in (2) in order to avoid the double account of the terms with $\mathbf{q} = 0$ at $\mathbf{p} = \mathbf{k}$.

Taking into account that, obviously, $V_{\mathbf{q}} = V_{-\mathbf{q}}$, equation $[\hat{H}_{diag}, b_{\mathbf{p}}^+] = \tilde{t}_{\mathbf{p}} b_{\mathbf{p}}^+$ leads to the following expression for $\tilde{t}_{\mathbf{p}}$:

$$\tilde{t}_{\mathbf{p}} = t_{\mathbf{p}} + \Omega^{-1} \sum_{\mathbf{k}} \frac{V_0 + V_{\mathbf{k}-\mathbf{p}}}{1 + \delta_{\mathbf{p}}^{\mathbf{k}}} n_{\mathbf{k}},\tag{3}$$

where $n_{\mathbf{k}}$ is the number of particles in a state with a momentum \mathbf{k} . At zero temperature we obtain:

$$\tilde{t}_{\mathbf{p}} = t_{\mathbf{p}} + c \frac{V_0 + V_{\mathbf{p}}}{1 + \delta_{\mathbf{p}}^0}, \quad (4)$$

where $c = N/\Omega$ is the concentration of atoms in the system. When we obtained (4), we assumed that at zero temperature all the atoms are in a state with a momentum $\mathbf{k} = 0$, because this approximation takes into account only the diagonal terms.

Obviously, $V_0 \geq 0$: otherwise, the system would be unstable [1]. On the other hand, $V_{\mathbf{q}}$ is the regular function of the parameter \mathbf{q} . So, we obtain the gap $\Delta_0 = V_0 c$ in the spectrum of one-atom excitations of the system.

When Bogolyubov obtained this result, he thought that it was the result of a wrong description of the system. Let us consider in more detail the reason why Bogolyubov considered the appearance of the gap in the spectrum of one-atom excitations a wrong solution.

Analysis of article [4] shows that Bogolyubov expected $\lim_{p \rightarrow 0} \tilde{t}_{\mathbf{p}}/p$ to coincide with the sound speed in the system and thus have a finite value. However, there is no physical principle, from which it would follow that the rate of one-atom excitations and the speed of the sound in the boson system should be equal, because the phonons and one-atom excitations are two various physical entities. To clarify this point it is sufficient to consider the system above the transition point.

As for the other arguments of Bogolyubov, they are secondary and required to explain why the obtained solution, from his point of view, was wrong. These arguments come down to the fact that the perturbation theory becomes inapplicable at small excitation momenta. We think that this argument are unjustified, because it is easy to show that the appearance of the gap in the one-atom excitation spectrum makes the calculation of the spectrum on the basis of the perturbation theory at small excitation momenta more robust. Indeed, the diagonal part of Hamiltonian \hat{V} , which, in fact, is responsible for the appearance of the gap, can be included in the so-called principle Hamiltonian of the perturbation theory. Accordingly, if this fact is taken into account, the absolute value of the appearing energy denominators turns out to be not less than the value $\sim \Delta_{\mathbf{p}} = V_{\mathbf{p}} c$, which makes the mentioned calculation more robust.

III. PHONONS AND ONE-ATOM EXCITATIONS IN THE PROPOSED APPROACH

Let us consider an elastic medium, the quantum oscillations of which correspond to creation and annihilation operators $\tilde{h}_{\mathbf{q}}^+$ and $\tilde{h}_{\mathbf{q}}$. This leads to a new term \hat{H}_{ph} to be added to the system Hamiltonian:

$$\hat{H}_{ph} = \sum_{\mathbf{q}} s q h_{\mathbf{q}}^+ h_{\mathbf{q}}, \quad (5)$$

where s - is the speed of the sound in the elastic medium thus introduced. Let us name hereafter the quantum oscillations of the elastic medium corresponding to the operators $\tilde{h}_{\mathbf{q}}^+$ and $\tilde{h}_{\mathbf{q}}$ seed phonons.

Let us introduce formally transformations corresponding to the procedure of renormalization of the atom-phonon interaction:

$$\begin{aligned}
b_{\mathbf{p}}^+ &= \tilde{b}_{\mathbf{p}}^+ - \Omega^{-1/2} \sum_{\mathbf{q} \neq 0} \varphi_{\mathbf{q}}^{\mathbf{p}} \tilde{b}_{\mathbf{p}-\mathbf{q}}^+ \tilde{h}_{\mathbf{q}}^+ + \Omega^{-1/2} \sum_{\mathbf{q} \neq 0} \varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}*} \tilde{b}_{\mathbf{p}+\mathbf{q}}^+ \tilde{h}_{\mathbf{q}} - \frac{1}{2} \Omega^{-1} \sum_{\mathbf{q} \neq 0} |\varphi_{\mathbf{q}}^{\mathbf{p}}|^2 \tilde{b}_{\mathbf{p}}^+ \\
&+ \frac{1}{2} \Omega^{-1} \sum_{\mathbf{k}, \mathbf{q} \neq 0} (\varphi_{-\mathbf{q}}^{\mathbf{p}-\mathbf{q}*} \varphi_{-\mathbf{q}}^{\mathbf{k}} - \varphi_{\mathbf{q}}^{\mathbf{k}+\mathbf{q}*} \varphi_{\mathbf{q}}^{\mathbf{p}}) \tilde{b}_{\mathbf{p}-\mathbf{q}}^+ \tilde{b}_{\mathbf{k}+\mathbf{q}}^+ \tilde{b}_{\mathbf{k}} \\
&- \frac{1}{2} \Omega^{-1} \sum_{\mathbf{k} \neq 0, \mathbf{q} \neq 0} (\varphi_{\mathbf{q}}^{\mathbf{p}-\mathbf{k}+\mathbf{q}*} \varphi_{\mathbf{k}}^{\mathbf{p}} + \varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}*} \varphi_{\mathbf{k}}^{\mathbf{p}+\mathbf{q}}) \tilde{b}_{\mathbf{p}+\mathbf{q}-\mathbf{k}}^+ \tilde{h}_{\mathbf{k}}^+ \tilde{h}_{\mathbf{q}} \\
&+ \frac{1}{4} \Omega^{-1} \sum_{\mathbf{k} \neq 0, \mathbf{q} \neq 0} (\varphi_{\mathbf{q}}^{\mathbf{p}-\mathbf{k}} \varphi_{\mathbf{k}}^{\mathbf{p}} + \varphi_{\mathbf{k}}^{\mathbf{p}-\mathbf{q}} \varphi_{\mathbf{q}}^{\mathbf{p}}) \tilde{b}_{\mathbf{p}-\mathbf{k}-\mathbf{q}}^+ \tilde{h}_{\mathbf{k}}^+ \tilde{h}_{\mathbf{q}}^+ \\
&+ \frac{1}{4} \Omega^{-1} \sum_{\mathbf{k} \neq 0, \mathbf{q} \neq 0} (\varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}*} \varphi_{\mathbf{k}}^{\mathbf{p}+\mathbf{q}+\mathbf{k}*} + \varphi_{\mathbf{k}}^{\mathbf{p}+\mathbf{k}*} \varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}+\mathbf{k}*}) \tilde{b}_{\mathbf{p}+\mathbf{q}+\mathbf{k}}^+ \tilde{h}_{\mathbf{k}} \tilde{h}_{\mathbf{q}},
\end{aligned} \tag{6}$$

$$\begin{aligned}
h_{\mathbf{q}}^+ &= \tilde{h}_{\mathbf{q}}^+ + \Omega^{-1/2} \sum_{\mathbf{p}} \varphi_{\mathbf{q}}^{\mathbf{p}*} \tilde{b}_{\mathbf{p}}^+ \tilde{b}_{\mathbf{p}-\mathbf{q}} \\
&+ \frac{1}{2} \Omega^{-1} \sum_{\mathbf{p}, \mathbf{k} \neq 0} (\varphi_{\mathbf{q}}^{\mathbf{p}*} \varphi_{\mathbf{k}}^{\mathbf{p}-\mathbf{q}+\mathbf{k}} - \varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{k}*} \varphi_{\mathbf{k}}^{\mathbf{p}+\mathbf{k}}) \tilde{h}_{\mathbf{k}}^+ \tilde{b}_{\mathbf{p}}^+ \tilde{b}_{\mathbf{p}+\mathbf{k}-\mathbf{q}} \\
&+ \frac{1}{2} \Omega^{-1} \sum_{\mathbf{p}, \mathbf{k} \neq 0} (\varphi_{\mathbf{q}}^{\mathbf{p}-\mathbf{k}*} \varphi_{\mathbf{k}}^{\mathbf{p}*} - \varphi_{\mathbf{k}}^{\mathbf{p}-\mathbf{q}*} \varphi_{\mathbf{q}}^{\mathbf{p}*}) \tilde{h}_{\mathbf{k}} \tilde{b}_{\mathbf{p}}^+ \tilde{b}_{\mathbf{p}-\mathbf{k}-\mathbf{q}}.
\end{aligned} \tag{7}$$

Operators \tilde{b}^+ , \tilde{b} , \tilde{h}^+ and \tilde{h} introduced in (6-7) are consistent with the standard commutation relations for bosons with a precision of $\sim \varphi^3$. Parameter φ in this approach plays the role of a formal small parameter.

In RPA approximation we formulate the equation on the transformation parameters such a way that the system Hamiltonian in terms of operators \tilde{b}^+ , \tilde{b} , \tilde{h}^+ and \tilde{h} would not include terms of the structure $\tilde{h}^+ \tilde{b}^+ \tilde{b}$ and $\tilde{h} \tilde{b}^+ \tilde{b}$. This equation will be of the form:

$$-V_{\mathbf{q}} J_{\mathbf{q}} + (t_{\mathbf{p}-\mathbf{q}} - t_{\mathbf{p}} + s q) \varphi_{\mathbf{q}}^{\mathbf{p}} + V_{\mathbf{q}} |J_{\mathbf{q}}|^2 \varphi_{\mathbf{q}}^{\mathbf{p}} + V_{\mathbf{q}} J_{\mathbf{q}}^2 \varphi_{-\mathbf{q}}^{\mathbf{p}-\mathbf{q}*} = 0, \tag{8}$$

where

$$J_{\mathbf{q}} = \Omega^{-1} \sum_{\mathbf{p}} (\varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}} - \varphi_{\mathbf{q}}^{\mathbf{p}}) n_{\mathbf{p}}, \tag{9}$$

and $n_{\mathbf{p}}$ is the thermodynamic average of the number of atoms in the state with a momentum \mathbf{p} . In (8) the numerical coefficient with terms $\sim V_{\mathbf{q}} |J_{\mathbf{q}}|^2$, $\sim V_{\mathbf{q}} J_{\mathbf{q}}^2$ was chosen in such a way that the spectrum calculated in the procedure of renormalization (see (15)) coincides with the spectrum of sound obtained on the basis of analysis of the spectral dependence of the system dielectric function [5]. Actually, in this case, we simply use the opportunity of choosing the order in which the terms are considered in a situation where the system is missing a real small parameter.

A nontrivial solution of equations (6-7) under the assumption that parameter $\varphi_{\mathbf{q}}^{\mathbf{p}}$ is real-valued is given below:

$$\varphi_{\mathbf{q}}^{\mathbf{p}} = \frac{J_{\mathbf{q}} V_{\mathbf{q}} (t_{\mathbf{p}} - t_{\mathbf{p}-\mathbf{q}} + s q)}{\omega_{\mathbf{q}}^2 - (t_{\mathbf{p}} - t_{\mathbf{p}-\mathbf{q}})^2}, \tag{10}$$

$$J_q^2 = \frac{\omega_q^2 - s^2 q^2}{2sqV_q}. \quad (11)$$

At that, ω_q is consistent with the following equation:

$$1 + \Omega^{-1} \sum_{\mathbf{p}} V_q \frac{n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{q}}}{t_{\mathbf{p}+\mathbf{q}} - t_{\mathbf{p}} + \omega_q} = 0. \quad (12)$$

Thus, the dependence of ω_q gives a sound spectrum obtained by analyzing the dielectric function of the system.

Kinetic terms \hat{H}_{ph}^{kin} contributing to the renormalization of energy of the seed phonons calculated with the use of RPA are of the form:

$$\hat{H}_{ph}^{kin} = \sum_{\mathbf{q}} sq \tilde{h}_{\mathbf{q}}^+ \tilde{h}_{\mathbf{q}} + \hat{H}_V + \hat{H}_t, \quad (13)$$

where

$$\begin{aligned} \hat{H}_V &= \sum_{\mathbf{q}} V_q J_q^2 \tilde{h}_{\mathbf{q}}^+ \tilde{h}_{\mathbf{q}} + \frac{1}{2} \sum_{\mathbf{q}} V_q J_q^2 \tilde{h}_{\mathbf{q}}^+ \tilde{h}_{-\mathbf{q}}^+ + \frac{1}{2} \sum_{\mathbf{q}} V_q J_q^2 \tilde{h}_{\mathbf{q}} \tilde{h}_{-\mathbf{q}}, \\ \hat{H}_t &= \Omega^{-1} \sum_{\mathbf{p}, \mathbf{q}} \left((t_{\mathbf{p}+\mathbf{q}} - t_{\mathbf{p}} - sq) |\varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}}|^2 + (t_{\mathbf{p}-\mathbf{q}} - t_{\mathbf{p}} + sq) |\varphi_{\mathbf{q}}^{\mathbf{p}}|^2 \right) n_{\mathbf{p}} \tilde{h}_{\mathbf{q}}^+ \tilde{h}_{\mathbf{q}} \\ &+ \Omega^{-1} \sum_{\mathbf{p}, \mathbf{q}} (t_{\mathbf{p}} - t_{\mathbf{p}+\mathbf{q}}) \varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}} \varphi_{-\mathbf{q}}^{\mathbf{p}} n_{\mathbf{p}} \tilde{h}_{\mathbf{q}}^+ \tilde{h}_{-\mathbf{q}}^+ \\ &+ \Omega^{-1} \sum_{\mathbf{p}, \mathbf{q}} (t_{\mathbf{p}} - t_{\mathbf{p}+\mathbf{q}}) \varphi_{\mathbf{q}}^{\mathbf{p}+\mathbf{q}} \varphi_{-\mathbf{q}}^{\mathbf{p}} n_{\mathbf{p}} \tilde{h}_{\mathbf{q}} \tilde{h}_{-\mathbf{q}}. \end{aligned} \quad (14)$$

For clarity we will first take into account only the contribution of \hat{H}_V to \hat{H}_{ph}^{kin} , which, actually, as is shown below, corresponds to the calculation of the spectrum in the long-wave limit. Diagonalization of the operator \hat{H}_{ph}^{kin} in this case using the Bogolyubov transformation leads to the following expression for the renormalized energy of the seed phonons $\varepsilon_{\mathbf{q}}$:

$$\varepsilon_{\mathbf{q}} = \omega_{\mathbf{q}}, \quad (15)$$

As is expected, the spectrum of the seed phonons coincides with the expression obtained for the spectrum of sound vibrations by calculating the dielectric function. In particular, for the Bose gas at zero temperature $\omega_{\mathbf{q}}$ coincides with the well-known expression obtained by Bogolyubov for the spectrum of quasiparticles [1] with neglect of the difference between the squared absolute value of the so-called Bogolyubov c - number and the full number of atoms in the system, i.e. we have:

$$\varepsilon_{\mathbf{q}} = \sqrt{t_{\mathbf{q}}(t_{\mathbf{q}} + 2\Delta_{\mathbf{q}})}. \quad (16)$$

The resulting expressions for the renormalized quantities in the suggested approach should be taken in the limit $s \rightarrow 0$. Indeed, in this case \hat{H}_{ph} does not add terms to the system Hamiltonian. So, the system of seed phonons only gives a set of states, which are used for the quantization of its oscillations. In particular, for the additional term of interatomic interaction $\delta\hat{V}$ following from the terms of Hamiltonian \hat{T} and \hat{H}_{ph} , we can obtain:

$$\delta\hat{V} = \frac{1}{2} \Omega^{-1} \sum_{\mathbf{p}, \mathbf{k}, \mathbf{q}} \delta V_{\mathbf{q}}^{\mathbf{p}, \mathbf{k}} \tilde{b}_{\mathbf{p}+\mathbf{q}}^+ \tilde{b}_{\mathbf{k}-\mathbf{q}}^+ \tilde{b}_{\mathbf{k}} \tilde{b}_{\mathbf{p}}, \quad (17)$$

where

$$\delta V_{\mathbf{q}}^{\mathbf{p},\mathbf{k}} = -\frac{1}{4}V_{\mathbf{q}} \frac{\omega_{\mathbf{q}}^2 \left[(t_{\mathbf{p}+\mathbf{q}} - t_{\mathbf{p}})^2 + (t_{\mathbf{k}} - t_{\mathbf{k}-\mathbf{q}})^2 \right]}{\left(\omega_{\mathbf{q}}^2 - (t_{\mathbf{p}+\mathbf{q}} - t_{\mathbf{p}})^2 \right) \left(\omega_{\mathbf{q}}^2 - (t_{\mathbf{k}} - t_{\mathbf{k}-\mathbf{q}})^2 \right)}. \quad (18)$$

Considering equation (18) leads (in the limit $p, k \rightarrow 0$) to the conclusion that renormalization does not contribute to the size of the gap in the one-atom excitation spectrum.

Now let us take into account also the contribution of \hat{H}_t in the spectrum of the phonons for the case of zero temperature. A simple calculation gives the following expression (compare with (15)):

$$\varepsilon_{\mathbf{q}} = \omega_{\mathbf{q}} \sqrt{1 + \frac{t_{\mathbf{q}}}{2\Delta_{\mathbf{q}}}}. \quad (19)$$

In fact, one can say that in the system one more expansion parameter appears, which is equal to $t_{\mathbf{q}}/2\Delta_{\mathbf{q}}$. It can be assumed, therefore, that the spectrum of phonons ends at the values of wave vector \mathbf{q} corresponding to the condition $t_{\mathbf{q}} \sim 2\Delta_{\mathbf{q}}$. Recall in this context that the spectrum of phonons is also limited at the shortwave region when the Boltzmann distribution for the occupation numbers of the atomic energy levels is determined. Besides, at high temperatures $T > \Delta_{\mathbf{q}}/4$ equation (12) has no solution for $\omega_{\mathbf{q}}$.

The suggested method makes it possible in principle to obtain the properties of the system with any accuracy, if one does not take into account the arbitrariness in the order of consideration of the terms appearing in the renormalization procedure. This arbitrariness is caused by the lack of a real small parameter in the system. We plan to eliminate it by comparison with the results of alternative methods of system's investigation.

Of course, not all the renormalized values will be calculated so simply as the correction to interatomic interaction energy $\delta\hat{V}$, because transformation parameter $\varphi_{\mathbf{q}}^{\mathbf{p}}$ has a singularity at $s \rightarrow 0$. At the same time, it seems that this problem is not of a fundamental nature. It is sufficient to increase the accuracy of transformations (6-7). At that, the appearing singular expressions will be reduced leaving only the finite values in the calculation results.

In summary, one can assert that at this stage of development of the suggested approach no reasons can be seen why the coexistence of the two branches of the excitation spectrum of the system may be doubted at temperatures below the transition point. It is quite another matter that the results obtained in the context of the suggested approach should be confirmed by other methods. Of course, in this case we mean a description of the system with the use of the technique of Green functions modified as compared with [6]. This technique should not break the fundamental symmetries of the system. We plan to perform such consideration in near future.

IV. BOSE GAS THERMODYNAMICS OF ONE-ATOM EXCITATIONS WITH INTERACTION

Now let us consider the case of finite temperatures assuming that they are sufficiently low to carry out the condition

$$\sum_{\mathbf{k} \neq 0} V_{\mathbf{k}-\mathbf{p}} n_{\mathbf{k}} \approx V_{\mathbf{p}} N_e, \quad (20)$$

where N_e is the full number of atoms in the excited states. In this case the simplification of (3) gives the following expressions:

$$\begin{aligned}\tilde{t}_0 &= 2\Delta_0 - \kappa\Delta_0, \\ \tilde{t}_{\mathbf{p}} &= t_{\mathbf{p}} + 2\Delta_0 + (\Delta_{\mathbf{p}} - \Delta_0) \{ \text{at } \mathbf{p} \neq 0 \},\end{aligned}\tag{21}$$

where κ is the fraction of atoms condensed in the ground orbital.

Let us assume that in the case of thermally activated atoms it is possible to use the parabolic dispersion law with a mass M_e , that is

$$\tilde{t}_{\mathbf{p}} \approx 2\Delta_0 + \frac{p^2}{2M_e}\tag{22}$$

at $\mathbf{p} \neq 0$. This simplification is possible, because $V_{\mathbf{p}} - V_0 \sim p^2$ at $\mathbf{p} \rightarrow 0$.

As for the system energy E , using the expression for \hat{H}_{diag} gives:

$$E = \sum_{\mathbf{p}} t_{\mathbf{p}} n_{\mathbf{p}} + \frac{V_0}{2\Omega} \sum_{\mathbf{p}} n_{\mathbf{p}} (n_{\mathbf{p}} - 1) + \frac{1}{2}\Omega^{-1} \sum_{\mathbf{p} \neq \mathbf{k}} (V_0 + V_{\mathbf{k}-\mathbf{p}}) n_{\mathbf{p}} n_{\mathbf{k}}\tag{23}$$

Again, assuming that the temperatures are sufficiently low to satisfy the conditions

$$\sum_{\mathbf{k} \neq 0, \mathbf{p} \neq 0, \mathbf{p} \neq \mathbf{k}} V_{\mathbf{k}-\mathbf{p}} n_{\mathbf{p}} n_{\mathbf{k}} \approx V_0 \sum_{\mathbf{k} \neq 0, \mathbf{p} \neq 0, \mathbf{p} \neq \mathbf{k}} n_{\mathbf{p}} n_{\mathbf{k}} \approx V_0 N_e^2,\tag{24}$$

it is possible to calculate energy ε per one atom of the large system:

$$\varepsilon = \Delta_0 \left(1 - \frac{\kappa^2}{2} \right) + (1 - \kappa) \langle t \rangle_e,\tag{25}$$

where $\langle t \rangle_e$ is the average kinetic energy of the excited atoms of the system:

$$\langle t \rangle_e = N_e^{-1} \sum_{\mathbf{p} \neq 0} t_{\mathbf{p}} \langle n_{\mathbf{p}} \rangle,\tag{26}$$

For average occupation numbers $\langle n_{\mathbf{p}} \rangle$ the Bose-Einstein distribution function is applicable. Thus, we have:

$$\langle n_{\mathbf{p}} \rangle = \frac{1}{\exp((p^2/2M_e + \kappa\Delta_0)/T) - 1},\tag{27}$$

because we assume, as usual, that the value of the chemical potential of the system is very close to \tilde{t}_0 .

Pass from sums to integrals it is possible to obtain an equation for the fraction of condensed atoms:

$$\kappa = 1 - \frac{(2M_e T)^{3/2}}{4\pi^2 c} \int \frac{\sqrt{x} dx}{\exp(\kappa\Delta_0/T + x) - 1}\tag{28}$$

and an expression for $\langle t \rangle_e$:

$$\langle t \rangle_e = \frac{M_e}{M} T \frac{\int \frac{x\sqrt{x} dx}{\exp(\kappa\Delta_0/T + x) - 1}}{\int \frac{\sqrt{x} dx}{\exp(\kappa\Delta_0/T + x) - 1}}.\tag{29}$$

Accordingly, it becomes possible to compare experimental data with calculations based on the proposed scheme and to estimate the gap Δ_0 and mass M_e of the excited atoms of the system.

TABLE I: Basic data and calculation results for a temperature range 1.5 – 2.1K

T, K	1.5	1.6	1.7	1.8	1.9	2.0	2.1
$U_{tot}, \text{ cal/g [7]}$	0.071	0.112	0.176	0.252	0.351	0.484	0.662
$U_{ph}, \text{ cal/g [8]}$	0.046	0.068	0.095	0.129	0.170	0.219	0.276
$\kappa, \% [9]$	94.33	89.83	83.92	76.12	66.90	55.79	41.84
$U_{at}, \text{ cal/g}$	0.025	0.044	0.081	0.123	0.181	0.265	0.386
$\tilde{\Delta}, K$	0.19	0.08	0.04	0.01	-	-	-
$\tilde{\gamma}$	0.43	0.52	0.63	0.70	-	-	-

V. DETERMINATION OF MODEL PARAMETERS BASED ON EXPERIMENTAL DATA WITH THE USE OF ENTHALPY AND THE FRACTION OF THE SF COMPONENT IN HE II

The calculation idea consists in the possibility of using two equations (25, 28) in order to determine two parameters Δ_0 and $\gamma = M_e/M$ at known values of temperature T , energy ε , and fraction of atoms condensed at the ground orbital κ .

The value of energy ε per one atom of helium can be obtained from the data of Kapitsa on the temperature dependence of enthalpy [7], because under the conditions of an isobaric experiment it is very close in value to the temperature dependence of the internal energy of the system. Indeed, pressure in the experiments of Kapitsa does not exceed 25 atm. So, the difference between the enthalpy of helium at zero and finite temperatures is very close in value to the difference of the corresponding internal energy values, because density changes in He II caused by temperature are very small.

According to the proposed concept the total enthalpy of the system determined in the experiment is a sum of two contributions: phonon - roton and one-atom excitations. Now we have a task of extraction the contribution of one-atom excitations from the total energy of the system.

The phonon contribution to the internal energy of the system is connected with the temperature dependence of the phonon heat capacity by the relation:

$$U_{ph}(T) = \int_0^T C_{ph}(t) dt. \quad (30)$$

At that, there is the well-known expression [8] for the heat capacity $C_{ph}(t)$:

$$C_{ph}(t) = \frac{2\pi^2}{15} k_B \left(\frac{k_B t}{\hbar S} \right)^3 + k_B \frac{p_0^2 \sqrt{\mu_r k_B t/2}}{\pi^{3/2} \hbar^3} \left(\frac{\Delta_r^2}{k_B^2 t^2} + \frac{\Delta_r}{k_B t} + \frac{3}{4} \right) \exp \left(-\frac{\Delta_r}{k_B t} \right), \quad (31)$$

where k_B - is Boltzmann constant. Nowadays experimental values of the phonon spectrum parameters used in (31)

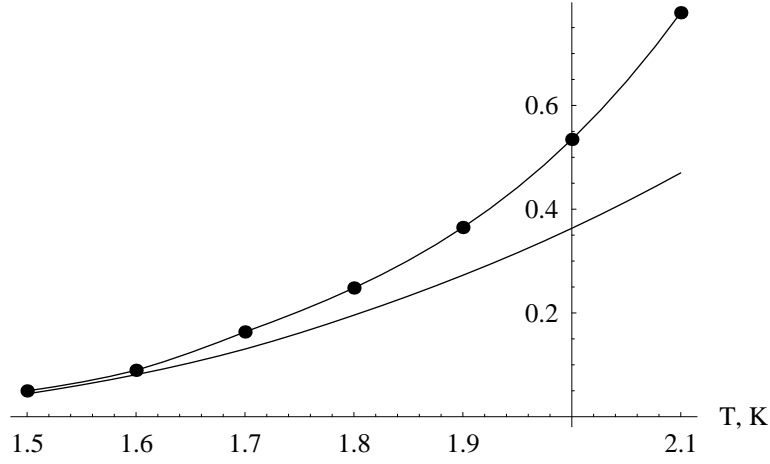


FIG. 1: Temperature dependence of one-atom excitation energy $\delta\varepsilon$ calculated from atomic energy U_{at} per one helium atom (upper curve). Besides, a calculated curve for the dependence $\delta\varepsilon(T)$ on the basis of (34) at selected values of Δ_0 and γ determined by (36) is presented (lower curve). All data are given in Kelvins.

are as follows:

$$\begin{aligned}
 S &= 2.38 \cdot 10^4 \text{ cm/sec}, \\
 \Delta_r &= 8.6 \text{ K}, \\
 p_0 &= 1.8 \cdot 10^8 \text{ h/cm}, \\
 \mu_r &= 0.13 M.
 \end{aligned} \tag{32}$$

Obviously, within the limits of a simple model of two branches of excitations one-atom excitation energy $U_{at}(T)$ can be obtained by simple subtraction of the phonon-roton contribution from the total energy of the system $U_{tot}(T)$:

$$U_{at}(T) = U_{tot}(T) - U_{ph}(T). \tag{33}$$

Temperature dependence of the fraction of condensed atoms in the ground state $\kappa(T)$ can be directly obtained from the results of an experiment by Andronikashvili (measuring the period of axial-torsion oscillations of a vessel filled with He II [9], or that by Peshkov (measuring the speed of second sound [10]). Both experiments give very similar dependencies $\kappa(T)$. It is relevant to note that the fundamentals of the phenomenological theory of He II, including the possibility of a two-fluid description of the system, cannot be doubted.

Table 1 presents the basic data for calculation of $U_{at}(T)$, as well as the results of calculations of other parameters that will be determined below. Fig. 1, respectively, presents the dependence of $\delta\varepsilon(T)$, value equal to energy $U_{at}(T)$ calculated per one atom of helium. Note here that the energy $\delta\varepsilon$, obviously, should be equal to energy ε , counted from its own value at $T = 0 \text{ K}$, i.e. (compare with (25))

$$\delta\varepsilon = \Delta_0 (1 - \kappa^2) / 2 + (1 - \kappa) \gamma T \frac{\int \frac{x \sqrt{x} dx}{\exp(\kappa \Delta_0 / T + x) - 1}}{\int \frac{\sqrt{x} dx}{\exp(\kappa \Delta_0 / T + x) - 1}}. \tag{34}$$

Dependencies $\tilde{\Delta}(T)$ and $\tilde{\gamma}(T)$ presented in the table are determined with the use of a self-consistent system of two

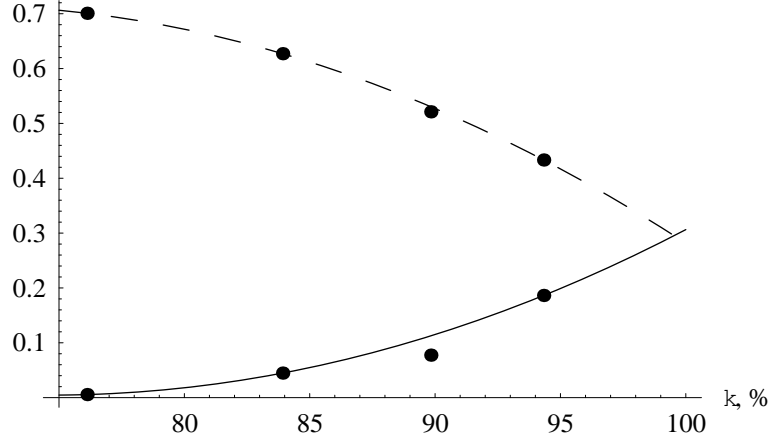


FIG. 2: Calculated dependencies $\tilde{\Delta}(\kappa)$ (solid curve, $\tilde{\Delta}$ are given in Kelvins) and $\tilde{\gamma}(\kappa)$ (dashed curve).

equations (compare with (25, 28))

$$\begin{aligned}
 \delta\varepsilon(T) &= \tilde{\Delta}(T) (1 - \kappa^2(T)) / 2 \\
 &+ (1 - \kappa(T)) \tilde{\gamma}(T) T \frac{\int \frac{x\sqrt{x}dx}{\exp(\kappa(T)\tilde{\Delta}(T)/(T+x)) - 1}}{\int \frac{\sqrt{x}dx}{\exp(\kappa(T)\tilde{\Delta}(T)/(T+x)) - 1}}, \\
 \kappa(T) &= 1 - \frac{(2\tilde{\gamma}(T)MT)^{3/2}}{4\pi^2c} \int \frac{\sqrt{x}dx}{\exp(\kappa(T)\tilde{\Delta}(T)/(T+x)) - 1}.
 \end{aligned} \tag{35}$$

The obtained dependencies $\tilde{\Delta}(T)$ and $\tilde{\gamma}(T)$ are the basis for obtaining the parameters Δ_0 and γ of the model. Indeed, when we deduced formula (25) we made the assumptions (20, 24)), which are realized the better the lower is the system temperature. On the other hand, it is difficult for us to estimate the temperature starting at which assumptions (20, 24) are realized with acceptable accuracy, because there are no reliable data on interatomic potentials. In this situation in order to obtain parameters Δ_0 and γ it is necessary to extrapolate dependencies $\tilde{\Delta}(T)$ and $\tilde{\gamma}(T)$ to the zero temperature range, where these assumptions are realized perfectly.

On the other hand, using the dependency $\kappa(T)$ enables to obtain the dependencies $\tilde{\Delta}(\kappa)$ and $\tilde{\gamma}(\kappa)$ shown in Fig. 2. At that, it becomes possible to extrapolate the obtained functions to the range of $\kappa = 1$. This also corresponds to the zero temperature case. This option seems to be more attractive, because the extrapolation becomes non-dimensional, and its value of $\approx 5\%$ seems to be small. Extrapolation parameters Δ_0 and γ obtained in this case have the following values:

$$\begin{aligned}
 \Delta_0 &= 0.31 \text{ K}, \\
 \gamma &= 0.28.
 \end{aligned} \tag{36}$$

It is obvious that dependency $\delta\varepsilon(T)$, calculated on the basis of (34) at the values of parameters Δ_0 and γ selected in (36) should approach dependency $\delta\varepsilon(T)$ calculated on the basis of (33) at decreasing temperature, because in this case correlations (20, 24) are realized better. Fig. 1 visualizes this statement.

VI. CALCULATION OF THE DIELECTRIC FUNCTION OF THE SYSTEM

When calculating the system response to an external action one should keep in mind the requirement of gradient invariance of the model. The below calculation takes into account this circumstance by using the well-known fact used for calculating the Hartree dielectric function: if Hamiltonian \hat{T} is taken as the basic Hamiltonian of the system, it is possible to calculate the response on the external potential with use of the standard theory of excitations. The Hamiltonian of this external potential \hat{U} has the form

$$\hat{U} = \int U(\mathbf{r}, t) b^+(\mathbf{r}) b(\mathbf{r}), \quad (37)$$

where $b^+(\mathbf{r})$ and $b(\mathbf{r})$ are creation and annihilation operators in coordinate representation. In this case the gradient symmetry of the system is not broken.

As one goes to a new basis of wave functions, in order to solve this problem in the context of the perturbation theory, a number of terms appear that have the same structure in RPA as the right hand side of equation (37). This circumstance is taken into account by introducing effective potential $U_{eff}(\mathbf{r}, t)$. At that, for Fourier transforms $U(\mathbf{r}, t)$ and $U_{eff}(\mathbf{r}, t)$ the following correlation exists:

$$U_{eff}(\mathbf{q}, \omega) = \frac{U(\mathbf{q}, \omega)}{\varepsilon_H(\mathbf{q}, \omega)}, \quad (38)$$

where $\varepsilon_H(\mathbf{q}, \omega)$ is the Hartree dielectric function:

$$\varepsilon_H(\mathbf{q}, \omega) = 1 + V_{\mathbf{q}} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{t_{\mathbf{k}+\mathbf{q}} - t_{\mathbf{k}} - (\omega + i0)}. \quad (39)$$

The presented procedure does not take into account the residual Hamiltonian \hat{H}_{res} , for which we have:

$$\hat{H}_{res} = \hat{V} + \hat{U} - \hat{U}_{eff}, \quad (40)$$

where

$$\hat{U}_{eff} = \int U_{eff}(\mathbf{r}, t) b^+(\mathbf{r}) b(\mathbf{r}) d\mathbf{r}. \quad (41)$$

In the new basis of wave functions, obtained after solving the Hartree problem of the perturbation theory, the matrix elements \hat{H}_{res} are invariant under the gradient transformation. Further let us restrict consideration to a simple case of the diagonal terms.

This consideration leads to a shift of the system energy levels. It turns to be important for determination of the occupation numbers $n_{\mathbf{k}}$ and $n_{\mathbf{k}+\mathbf{q}}$ in (39): calculating them one should use the Bose-Einstein distribution function, in which one-atom energies $\tilde{t}_{\mathbf{k}}$ and $\tilde{t}_{\mathbf{k}+\mathbf{q}}$ are used as energy levels.

Note one more feature of the Hamiltonian \hat{H}_{res} . Obviously, the response of the system on the Hamiltonian \hat{U}_{eff} described by the dielectric function at zero temperature corresponds to the response of an ideal SF fluid. At the same

time, non-diagonal, time-dependent terms of the Hamiltonian \hat{H}_{res} can lead to dissipation of energy due to transitions from the ground state to the excited ones if the frequency of the external action exceeds the gap energy in the one-atom excitation spectrum. Here it is reasonable to make a most general remark: the appearance of time-dependent non-diagonal terms of the Hamiltonian in the procedure of calculating the system response to an external action for the models using gapless one-atom excitation spectra can mean the appearance of an energy dissipation channel in the system, even if it satisfies the SF principles from a formal point of view.

On the other hand, the hypothetical possibility of the existence of a gap in the one-atom excitation spectrum of SF state has been suggested before [11, 12]. For such models it is possible to observe directly the gap size values. For example, if voltage is applied to a metal needle, then near its tip a force appears that exerts influence upon the helium atoms. Therefore, the conditions of the experiment proposed earlier in very general terms [12], become better defined, because now we know the frequency interval, in which a thorough investigation of the phase and amplitude-frequency characteristics of the chain which includes a sensor in the form of the above needle should be carried out.

VII. CONCLUSION

This paper suggests the SF model of He II preserving the fundamental symmetries of the system at all temperatures including those below the transition point. The structure of energy levels appearing in the model is determined by the possibility of coexistence of phonon and one-atom spectra below the transition point.

Numerical simulation showed satisfactory agreement of the model with the experimental data below the transition point. In particular, we succeeded in estimating the value of the gap in the one-atom excitation spectrum, which turned out to be approximately equal to 0.31 K at zero temperature. We suggest a method of direct observation of the gap in the one-atom excitation spectrum on basis of the data on energy absorption in the system under the influence of an external oscillating force.

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